

# Quaternary-singlet State of Spin-1 Bosons in Optical Lattice

Jie Zhang<sup>\*1</sup>

<sup>1</sup>College of Physics and optoelectronics, Taiyuan University of Technology, Taiyuan 030024, Shanxi, China

We present the quantum ground state properties of  $^{23}\text{Na}$  spinor condensates, which is confined in a periodic or double-well potential and subject to a magnetic dipole-dipole interaction between nearby wells. A novel singlet state arise in the system and can be discussed in explicit form. Caused by the competition between the intra-site spin exchange interactions and the inter-site dipole-dipole interactions, this quaternary-singlet state is a entangled state formed by at least four particles and vanish the total spin. This is distinct from the direct product of the two conventional singlet pairs.

PACS numbers: 03.75.Lm, 03.75.Mn, 67.85.Fg

## I. INTRODUCTION

The Heisenberg model of spin-spin interactions defined by  $H = J \sum_{\langle i,j \rangle} \mathbf{F}_i \cdot \mathbf{F}_j$  is often considered as the starting point for understanding many complex magnetic structures in solids such as ferromagnetism and antiferromagnetism at temperatures below the Curie temperature. This Hamiltonian arises from the direct Coulomb interaction among electrons and the Pauli exclusion principle, with  $\mathbf{F}_i$  the spin operator for the  $i$ th electron.

The study of bosonic spin-spin interactions rise since the success in trapping a  $^{23}\text{Na}$  condensate in an optical potential [1], where spin degrees of freedom are liberated and it give rise to a rich variety phenomena such as spin domain formations [2], spin mixing dynamics [3], topological defects and so on. The properties of such a three-component spinor condensate were first studied with atomic spin coupling interaction takes the form  $V(\mathbf{r}) = (c_0 + c_2 \mathbf{F}_1 \cdot \mathbf{F}_2) \delta(\mathbf{r})$  by Ho [4] and Ohmi [5], and had been implemented experimentally [2], where two different spin-dependent phases exist: the so-called antiferromagnetic and ferromagnetic states for  $^{23}\text{Na}$  and  $^{87}\text{Rb}$  atomic condensates respectively.

This spinor BECs can be confined in optical lattices, which offers a unique opportunity to study magnetic properties of matter with tunable parameters. The quantum phase transition from the superfluid phase to the Mott insulating state is well described by the spinless Bose-Hubbard Hamiltonian [6, 7] and was demonstrated in experiments [8, 9]. With the atomic spin coupling interaction involved, the Bose-Hubbard Hamiltonian is studied in the Mott insulating regime, where phase coherence or superfluidity is lost, and atoms are localized with number fluctuations suppressed. Such a insulating state represents a correlated many-body state of bosons and the calculations of the magnetic properties within spin-exchange interactions have been carried out sufficiently [10–16].

In addition to the spin-exchange interaction, there exists another important type of magnetic interaction, the magnetic dipole-dipole interaction [17–24], which plays an important role in domain formation in macroscopic samples. This model includes the long-range magnetic

dipole-dipole interaction between different lattice sites, but neglects it within each site [13], assuming that it is much weaker than the s-wave interaction described.

It is predicted that the ground state of  $^{23}\text{Na}$  BEC ( $c_2 > 0$ ) is a spin singlet with properties ( $n_1 = n_0 = n_{-1} = N/3$ ) [25] contrast with those of mean field prediction. Soon, Ho and Yip [26] show that this spin singlet state is a fragmented condensate with anomalously large number fluctuations and thus has fragile stability. The remarkable nature of this fragmentation is that the single particle reduced density matrix gives three macroscopic eigenvalues (above) with large number fluctuations  $\Delta n_{1,0,-1} \sim N$ . In this paper, we consider specifically the case of spinor  $^{23}\text{Na}$  condensates and discuss the ground state properties and quantum number fluctuations in the Zeeman components.

## II. THE MODEL HAMILTONIAN

The simple two well model Hamiltonian includes  $\hat{H} = \hat{H}_1 + \hat{H}_2 + \hat{H}_{12}$  where

$$\begin{aligned} \hat{H}_1 = \int d\mathbf{r} \left\{ \hat{\Psi}_\alpha^\dagger \left( \frac{\hbar^2}{2M_1} \nabla^2 + V_{trap} \right) \hat{\Psi}_\alpha + \frac{\alpha_1}{2} \hat{\Psi}_\alpha^\dagger \hat{\Psi}_\beta^\dagger \hat{\Psi}_\beta \hat{\Psi}_\alpha \right. \\ \left. + \frac{\beta_1}{2} \hat{\Psi}_\alpha^\dagger \hat{\Psi}_\beta^\dagger \mathbf{F}_{\alpha\nu} \cdot \mathbf{F}_{\beta\mu} \hat{\Psi}_\mu \hat{\Psi}_\nu \right\} \end{aligned} \quad (1)$$

is the in-site spinor BEC Hamiltonian [4, 5], the spin-dependent  $\delta$  interaction is  $V_\delta(\mathbf{r}) = (\alpha + \beta \mathbf{F} \cdot \mathbf{F}) \delta(\mathbf{r})$  with  $\alpha, \beta$  characterize the short-range spin-independent and spin-changing s-wave collisions, respectively.  $\hat{\mathbf{F}} = \hat{a}_\alpha^\dagger \mathbf{F}_{\alpha\beta} \hat{a}_\beta$  is defined in terms of the  $3 \times 3$  spin-1 matrices  $\mathbf{F}_{\alpha\beta}$ , and  $\alpha, \beta = 1, 0, -1$  describe the three Zeeman levels with repeated indices to be summed over.  $H_2$  is identical to  $H_1$  except for the substitution of subscript 1 by 2 and  $\hat{\Psi}_i$  by  $\hat{\Phi}_i$ .

The dipole-dipole Hamiltonian is

$$\hat{H}_{12} = \int d\mathbf{r} \hat{\Psi}_\alpha^\dagger \hat{\Phi}_\beta^\dagger V_{dd}(\mathbf{r}_1 - \mathbf{r}_2) \hat{\Phi}_\beta \hat{\Psi}_\alpha \quad (2)$$

with

$$V_{dd} = \frac{\mu_0}{4\pi} \left[ \frac{\mathbf{d}_1 \cdot \mathbf{d}_2}{|\mathbf{r}_{12}|^3} - \frac{3(\mathbf{d}_1 \cdot \hat{\mathbf{r}}_{12})(\mathbf{d}_2 \cdot \hat{\mathbf{r}}_{12})}{|\mathbf{r}_{12}|^3} \right] \quad (3)$$

$\mu_0$  the magnetic permeability of vacuum,  $\mathbf{d}_{1,2}=g_F\mu_B\mathbf{F}_{1,2}$  with  $g_F\mu_B$  the gyromagnetic ratio, and  $\mathbf{r}_{12} = \mathbf{r}_1 - \mathbf{r}_2$ ,  $\hat{\mathbf{r}}_{12} = \mathbf{r}_{12}/|\mathbf{r}_{12}|$ ,  $\mathbf{r}_{1,2}$  is the coordinate of the 1, 2 site.

We adopt the single model approximation [25, 27, 28] for each of the two spinor condensates in the nearby sites with modes  $\Psi(\mathbf{r})$  and  $\Phi(\mathbf{r})$ , i.e., setting

$$\hat{\Psi}_i = \hat{a}_i\Psi, \quad \hat{\Phi}_i = \hat{b}_i\Phi, \quad i = 1, 0, -1 \quad (4)$$

with  $\hat{a}_i$  ( $\hat{b}_i$ ) the annihilation operator for the ferromagnetic (polar) atoms satisfying  $[\hat{a}_i, \hat{a}_j] = 0$  and  $[\hat{a}_i, \hat{a}_j^\dagger] = \delta_{ij}$  (and the same form of commutations for  $\hat{b}_i$ ). substitute  $\hat{\Psi}_i, \hat{\Phi}_i$  into  $\hat{H}_1, \hat{H}_2$ . The spin-independent part can be reduced to a constant operator for a fix number of atoms  $N = N_1 + N_0 + N_{-1}$ ,

$$\begin{aligned} \left(\frac{\hbar^2}{2M_1}\nabla^2 + U_1 + \frac{\alpha_1}{2}N|\Psi|^2\right)\Psi &= \mu_1\Psi \\ \left(\frac{\hbar^2}{2M_2}\nabla^2 + U_2 + \frac{\alpha_2}{2}N|\Phi|^2\right)\Phi &= \mu_2\Phi \end{aligned} \quad (5)$$

here  $\mu_{1,2}$  is the mean field energy or the chemical potential in the two wells.

The spin-dependent Hamiltonian finely reduce to

$$\hat{H}_1 = C_1\hat{\mathbf{F}}_1^2, \quad \hat{H}_2 = C_2\hat{\mathbf{F}}_2^2, \quad (6)$$

with  $C_1 = \beta_1 \int d\mathbf{r} |\Psi(r)|^4$ ,  $C_2 = \beta_2 \int d\mathbf{r} |\Phi(r)|^4$ .

In the one-dimensional double well or optical lattice, according to the the vector subtraction,  $\mathbf{r}_{12} = \mathbf{r}_1 - \mathbf{r}_2$  always point at the only one direction. If we choose the quantization axis along this direction as z axis, the  $V_{dd}$  reduced to

$$\begin{aligned} V_{dd} &= \lambda[\mathbf{F}_1 \cdot \mathbf{F}_2 - 3(\mathbf{F}_1 \cdot \hat{\mathbf{r}}_{12})(\mathbf{F}_2 \cdot \hat{\mathbf{r}}_{12})] \\ &= \lambda[\mathbf{F}_1 \cdot \mathbf{F}_2 - 3\mathbf{F}_{1z}\mathbf{F}_{2z}] \end{aligned} \quad (7)$$

with  $\lambda = \frac{\mu_0(g_F\mu_B)^2}{4\pi|\mathbf{r}_{12}|^3}$ . The Hamiltonian  $\hat{H}_{12}$  finely reads

$$\hat{H}_{12} = \Lambda(\hat{\mathbf{F}}_1 \cdot \hat{\mathbf{F}}_2 - 3\hat{F}_{1z}\hat{F}_{2z}) \quad (8)$$

with  $\Lambda = \lambda \int d\mathbf{r} |\Psi(r)|^2 |\Phi(r)|^2$ .

The total Hamiltonian [20, 21] is

$$\hat{H} = C_1\hat{\mathbf{F}}_1^2 + C_2\hat{\mathbf{F}}_2^2 + \Lambda\hat{\mathbf{F}}_1 \cdot \hat{\mathbf{F}}_2 - 3\Lambda\hat{F}_{1z}\hat{F}_{2z} \quad (9)$$

In the absence of long-range magnetic dipole-dipole interaction or external magnetic fields, there is no spin correlations between sites. For the Rb<sup>87</sup> condensate, the ground state in the individual sites favors polarizing all the spins to the same direction, therefore they can be considered as independent “magnets” whose pseudospin vectors point in random directions. But for individual Na<sup>23</sup> condensate, they favors vanishing the total spin in each site. As  $\eta = \mu_0(g_F\mu_B)^2/4\pi|\mathbf{r}_{12}|^3$  can be greatly

enhanced by the light-induced optical dipolar interaction if one chooses appropriate laser fields to form the potential well [29, 30], we aim to determine the spin structure of the system if the different sites are allowed to interact with each other through the magnetic dipole-dipole interaction.

### III. THE GROUND STATE PROPERTIES

#### A. A brief review of singlet state

Without the magnetic dipole-dipole interaction or for the intra-site pure spin-1 condensate ( $\hat{H}_0 = C\hat{\mathbf{F}}^2$ ), the simplest ground state for the F=1 spinor <sup>23</sup>Na condensates ( $C > 0$ ) is a spin singlet formed by two spin-1 particles described as

$$|F, m\rangle = \sum_{m_1, m_2=1, 0, -1} G |F_1 = 1, m_1\rangle |F_2 = 1, m_2\rangle \quad (10)$$

with  $F = F_1 + F_2 = 0$  is the total spin,  $m = m_1 + m_2 = 0$  is the total z component,  $G$  is the Clebsch-Gordon coefficient.

$$|F, m\rangle = \frac{1}{\sqrt{3}}\hat{A}^\dagger |0\rangle \quad (11)$$

The operator  $\hat{A}^\dagger \equiv (\hat{a}_0^\dagger)^2 - 2\hat{a}_1^\dagger\hat{a}_{-1}^\dagger$  describe a singlet pair creating operator formed by two identical spin-1 bosons, and the ground state of N particles is  $(\hat{A}^\dagger)^{N/2} |0\rangle$ .  $G$  is the CG coefficient. The particle density matrix  $(\hat{\rho})_{\alpha\beta} = \langle \hat{a}_\alpha^\dagger \hat{a}_\beta \rangle$  is

$$\langle \hat{a}_\alpha^\dagger \hat{a}_\beta \rangle = \begin{pmatrix} N/3 & & \\ & N/3 & \\ & & N/3 \end{pmatrix} \quad (12)$$

with  $\alpha, \beta=1, 0, -1$ . This matrix has three equal macroscopic eigenvalues called “superfragmented state” [26]. A weak external magnetic field along z ( $\hat{H}_0 = C\hat{\mathbf{F}}^2 - p\hat{F}_z$ ) can break the pairs and polarize the system [31, 32] with the ground state described as

$$|F = S, m = S\rangle = (\hat{a}_1^\dagger)^S (\hat{A}^\dagger)^{(N-S)/2} |0\rangle \quad (13)$$

The particle numbers on the three Zeeman levels are re-distributed as

$$\begin{aligned} N_1 &= \frac{(N+S)(S+1)}{2S+3} + \frac{S}{2S+3} \\ N_{-1} &= \frac{(N-S)(S+1)}{2S+3} \\ N_0 &= \frac{N-S}{2S+3} \end{aligned}$$

with the 0-component distribution shrink rapidly as S increases.

### B. A brief review of dimmer state

For the subspace of exactly one particle per well, the Mott-insulator ground state of one-dimensional optical lattice has been confirmed to be a dimmer states[40] with the form,

$$\Psi_{dimer} = \Psi_{12}\Psi_{34}\Psi_{56}\dots \quad (14)$$

where the state

$$\begin{aligned} \Psi_{12} &= \frac{-1}{\sqrt{3}}(|1, -1\rangle + |-1, 1\rangle - |0, 0\rangle)_{12} \\ &= \frac{1}{\sqrt{3}}(\hat{a}_0^\dagger \hat{b}_0^\dagger - \hat{a}_1^\dagger \hat{b}_{-1}^\dagger - \hat{a}_{-1}^\dagger \hat{b}_1^\dagger) |0\rangle \\ &= \frac{1}{\sqrt{3}} \hat{\Theta}_{12}^\dagger |0\rangle \end{aligned} \quad (15)$$

The operator  $\hat{\Theta}_{12}^\dagger \equiv \hat{a}_0^\dagger \hat{b}_0^\dagger - \hat{a}_1^\dagger \hat{b}_{-1}^\dagger - \hat{a}_{-1}^\dagger \hat{b}_1^\dagger$  describe a singlet pair creating operator formed by two spin-1 bosons in the different site.

For more or at least two particles per well, the ground states are more complicated.

### C. The quaternary-singlet State

For simplify, we first consider  $3\Lambda\hat{F}_{1z}\hat{F}_{2z} = 0$ , which serves as reference case for the complete discussion.

$$\hat{H} = C_1\hat{\mathbf{F}}_1^2 + C_2\hat{\mathbf{F}}_2^2 + \Lambda\hat{\mathbf{F}}_1 \cdot \hat{\mathbf{F}}_2 \quad (16)$$

It can be rewrited as[33–39]

$$\hat{H} = a\hat{\mathbf{F}}_1^2 + b\hat{\mathbf{F}}_2^2 + c\hat{\mathbf{F}}^2, \quad (17)$$

with  $a = C_1 - \Lambda/2$ ,  $b = C_2 - \Lambda/2$ , and  $c = \Lambda/2$ ,  $\hat{\mathbf{F}} = \hat{\mathbf{F}}_1 + \hat{\mathbf{F}}_2$  is the total spin operator. The eigenstates of (17) are the common eigenstates for the commuting operators  $\hat{\mathbf{F}}_1^2$ ,  $\hat{\mathbf{F}}_2^2$ ,  $\hat{\mathbf{F}}^2$ , and  $\hat{F}_z$ , given by

$$|F_1, F_2, F, m\rangle = \sum_{m_1 m_2} C_{F_1, m_1; F_2, m_2}^{F, m} |F_1, m_1\rangle |F_2, m_2\rangle, \quad (18)$$

with the uncoupled basis states  $|F_1, m_1\rangle$  ( $|F_2, m_2\rangle$ ) generated from equation (13) by a repeat using lowering operator  $\hat{F}_{1-}$ , and they can span a Hilbert space of dimension  $(N_1 + 1)(N_1 + 2)/2$  [41].  $C$  is the Clebsch-Gordon coefficient. The corresponding eigenenergy is

$$E = aF_1(F_1 + 1) + bF_2(F_2 + 1) + cF(F + 1) \quad (19)$$

Given  $N_j$ , the allowed values of  $F_j$  are  $F_j = 0, 2, 4, \dots, N_j$  if  $N_j$  is even; and  $F_j = 1, 3, 5, \dots, N_j$  if  $N_j$  is odd, satisfying  $|F_1 - F_2| \leq F \leq F_1 + F_2$ .

We will next consider the special case of  $N_1 = N_2 = N$  and for  $N$  even.

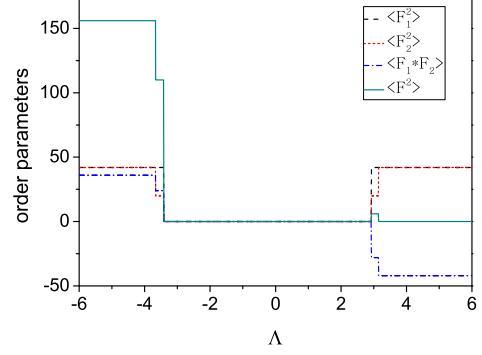


FIG. 1: (Color online) The dependence of ground-state order parameters on  $\Lambda$  at fixed values of  $C_1 = 1$ ,  $C_2 = 2$ , (in the unit of  $|C_1|$ ). Black dashed lines, red short dashed lines, blue dot-dashed lines and green solid lines denote respectively the order parameters  $\bar{\mathbf{F}}_1^2$ ,  $\bar{\mathbf{F}}_2^2$ ,  $\bar{\mathbf{F}}_1 \cdot \bar{\mathbf{F}}_2$ , and  $\bar{\mathbf{F}}^2$ .

Fig. 1 shows the development of the four order parameters

$$\begin{aligned} \bar{\mathbf{F}}_1^2 &= \langle \hat{\mathbf{F}}_1^2 \rangle, \\ \bar{\mathbf{F}}_2^2 &= \langle \hat{\mathbf{F}}_2^2 \rangle, \\ \bar{\mathbf{F}}_1 \cdot \bar{\mathbf{F}}_2 &= \langle \hat{\mathbf{F}}_1 \cdot \hat{\mathbf{F}}_2 \rangle, \\ \bar{\mathbf{F}}^2 &= \langle \hat{\mathbf{F}}^2 \rangle \end{aligned} \quad (20)$$

for  $\Lambda$  (in the unit of  $|C_1|$ ) with even particles per well (take  $N_1 = N_2 = 6$ ). We find that in the  $\Lambda < \frac{-(2N-1)C_2}{C_1N}$  region,  $\bar{\mathbf{F}}_1^2$ ,  $\bar{\mathbf{F}}_2^2$ , and  $\bar{\mathbf{F}}_1 \cdot \bar{\mathbf{F}}_2$  are all polarized to the maximum with the system being ferromagnetic. In the region  $\Lambda \in [-C_1 - C_2, C_1 + C_2]$ , the two sites are essentially independent for a weak inter-sites dipole-dipole interaction. This phase is a total spin singlet  $\bar{\mathbf{F}}^2 = 0$  described by the direct product of the polar ground state  $(\hat{A}^\dagger)^{N/2}(\hat{B}^\dagger)^{N/2}|0\rangle$  giving rise to  $\bar{\mathbf{F}}_1^2 = 0$ ,  $\bar{\mathbf{F}}_2^2 = 0$  and  $\bar{\mathbf{F}}_1 \cdot \bar{\mathbf{F}}_2 = 0$ . When  $\Lambda > \frac{(2N-1)C_2}{C_1(N+1)}$  they are polarized to the maximum but in the opposite directions with  $\bar{\mathbf{F}}^2 = 0$  and  $-2\bar{\mathbf{F}}_1 \cdot \bar{\mathbf{F}}_2 = \bar{\mathbf{F}}_1^2 + \bar{\mathbf{F}}_2^2 \neq 0$ . We find interestingly that in this state the total spin vanishes, while the sites spins satisfy  $\bar{\mathbf{F}}_1^2 = \bar{\mathbf{F}}_2^2 = N(N+1)$ .

The ground state in the region  $\Lambda > \frac{(2N-1)C_2}{C_1(N+1)}$  is a singlet, with all basis states obeying the condition  $m_1 + m_2 = 0$ . All channels of total spin zero have to be taken

into account and we have

$$|N, N, 0, 0\rangle = \sum_{m_1=-N}^N C_{N, m_1; N, -m_1}^{0, 0} |N, m_1\rangle |N, -m_1\rangle. \quad (21)$$

If we take  $N_1 = N_2 = 2$  for example, we find that

$$|2, 2, 0, 0\rangle = \frac{1}{2\sqrt{5}}((\hat{\Theta}_{12}^\dagger)^2 - \frac{1}{3}\hat{A}^\dagger \hat{B}^\dagger)|0\rangle \quad (22)$$

Compared to the “superfragmented state”  $(\hat{A}^\dagger)^{N/2} |0\rangle = ((\hat{a}_0^\dagger)^2 - 2\hat{a}_1^\dagger \hat{a}_{-1}^\dagger)^{N/2} |0\rangle$  [26], this quaternary-singlet states has the similar appearance. However it is not the direct product of the two conventional singlet pairs,  $|2, 2, 0, 0\rangle \neq \hat{A}^\dagger \hat{B}^\dagger |0\rangle$ . The difference between  $|N, N, 0, 0\rangle$  and  $(\hat{A}^\dagger)^{N/2} (\hat{B}^\dagger)^{N/2} |0\rangle$  can be easily find in the phase diagram (Fig.1).

#### D. The number fluctuations

We notice that

$$\begin{aligned} [\hat{\mathbf{F}}_1^2, \hat{\Theta}_{12}^\dagger \hat{\Theta}_{12}] &\neq 0, [\hat{\mathbf{F}}_2^2, \hat{\Theta}_{12}^\dagger \hat{\Theta}_{12}] \neq 0, \\ [\hat{\mathbf{F}}^2, \hat{\Theta}_{12}^\dagger \hat{\Theta}_{12}] &= 0 \end{aligned} \quad (23)$$

and it is easy to understand that  $\hat{\mathbf{F}}^2 (\hat{\Theta}_{12}^\dagger)^N |0\rangle = 0$ . In this section, we will talk about three different singlet states, the quaternary-singlet state  $|N, N, 0, 0\rangle$ , the dimer state  $(\hat{\Theta}_{12}^\dagger)^N |0\rangle$  and the direct product singlet state  $(\hat{A}^\dagger)^{N/2} (\hat{B}^\dagger)^{N/2} |0\rangle$ , the properties such as

$$\hat{\mathbf{F}}^2 (\hat{A}^\dagger)^{N_1} (\hat{B}^\dagger)^{N_2} |0\rangle = 0, \hat{\mathbf{F}}^2 |N, N, 0, 0\rangle = 0 \quad (24)$$

are shown in Fig.1.

As a exceptional case, all eigenvectors  $|N, m_1\rangle$  in (18) can be expressed in terms of the Fock states [42], which are defined as

$$\begin{aligned} \hat{n}_\alpha^{(j)} |n_1^{(j)}, n_0^{(j)}, n_{-1}^{(j)}\rangle &= n_\alpha^{(j)} |n_1^{(j)}, n_0^{(j)}, n_{-1}^{(j)}\rangle, \\ \alpha &= 0, \pm 1; j = 1, 2 \end{aligned} \quad (25)$$

For the state  $|N, N, 0, 0\rangle$ , we calculate the particle numbers and number fluctuations on the Fock states and find that the average numbers of atoms in the six components are exactly all equal,  $\langle n_1^{(j)} \rangle = \langle n_0^{(j)} \rangle = \langle n_{-1}^{(j)} \rangle = N/3$ . The fluctuations are given explicitly

$$\begin{aligned} \langle \Delta n_0^{(j)} \rangle &= \frac{\sqrt{N^2 + 9N}}{3\sqrt{5}} \\ \langle \Delta n_{\pm 1}^{(j)} \rangle &= \frac{2\sqrt{N^2 + 3N/2}}{3\sqrt{5}} \end{aligned} \quad (26)$$

which approximatively satisfy  $\langle \Delta n_1^{(j)} \rangle = 2 \langle \Delta n_0^{(j)} \rangle = \langle \Delta n_{-1}^{(j)} \rangle$  for large  $N$  [36], as opposed to  $2 \langle \Delta n_1 \rangle = \langle \Delta n_0 \rangle = 2 \langle \Delta n_{-1} \rangle$  for the single species or intra-site singlet state ( $C_{1,2} > 0$ ) [26].

The difference between these states are obvious. As total spin  $F$  vanishes, the number distributions are all  $\langle n_1^{(j)} \rangle = \langle n_0^{(j)} \rangle = \langle n_{-1}^{(j)} \rangle = N/3$ , but the number fluctuation distribution in these states are quite different, it has been shown that for the state  $Z^{1/2} (\hat{A}^\dagger)^{N_1} (\hat{B}^\dagger)^{N_2} |0\rangle$

[26], they are

$$\begin{aligned} \langle \Delta n_1^{(j)} \rangle &= \langle \Delta n_0^{(j)} \rangle / 2 = \langle \Delta n_{-1}^{(j)} \rangle \\ &= \frac{\sqrt{N^2 + 3N}}{3\sqrt{5}} \end{aligned} \quad (27)$$

For the state  $Z^{1/2} (\hat{\Theta}_{12}^\dagger)^N |0\rangle$ , according to the multinomial theorem

$$(x_1 + x_2 + x_3)^n = \sum_{k=0}^n \sum_{l=0}^k c_{nlk} x_1^{n-k} x_2^{k-l} x_3^l \quad (28)$$

with  $c_{nlk} = n! / (l!(k-l)!(n-k)!)$ , we find that the state  $(\hat{\Theta}_{12}^\dagger)^N |0\rangle$  can be described by the Fock state  $|n_1^{(1)}, n_0^{(1)}, n_{-1}^{(1)}\rangle \otimes |n_1^{(2)}, n_0^{(2)}, n_{-1}^{(2)}\rangle$  as

$$\begin{aligned} (\hat{\Theta}_{12}^\dagger)^N |0\rangle &= (\hat{a}_0^\dagger \hat{b}_0^\dagger - \hat{a}_1^\dagger \hat{b}_{-1}^\dagger - \hat{a}_{-1}^\dagger \hat{b}_1^\dagger)^N |0\rangle \\ &= \sum_{k=0}^N \sum_{l=0}^k c_{Nlk} (\hat{a}_0^\dagger \hat{b}_0^\dagger)^{N-k} (-\hat{a}_1^\dagger \hat{b}_{-1}^\dagger)^{k-l} (-\hat{a}_{-1}^\dagger \hat{b}_1^\dagger)^l |0\rangle \\ &= \sum_{k=0}^N \sum_{l=0}^k (-1)^k N! |k-l, N-k, l\rangle \otimes |l, N-k, k-l\rangle \end{aligned} \quad (29)$$

where we have used the property  $(\hat{a}^\dagger)^N |0\rangle = \sqrt{N!} |N\rangle$ . We find that the number fluctuations are equally distributed, i.e.

$$\begin{aligned} \langle \Delta n_1^{(j)} \rangle &= \langle \Delta n_0^{(j)} \rangle = \langle \Delta n_{-1}^{(j)} \rangle \\ &= \sqrt{N(N+1)/6 - N^2/9} \end{aligned} \quad (30)$$

#### E. The term $3\Lambda \hat{F}_{1z} \hat{F}_{2z}$

For the real Hamiltonian (9), the last term plays an important role in domain formation and can polarize the spin to the same direction. This interaction offers a effect extra uniform weak field to the nearby site and breaks the singlet states. The ground state can be constructed using the quaternary-singlet state  $|N, N, 0, 0\rangle$  and direct product singlet state  $(\hat{A}^\dagger)^{N/2} (\hat{B}^\dagger)^{N/2} |0\rangle$ .

In the region  $\Lambda \in [-C_1 - C_2, C_1 + C_2]$ , since the spin singlet operator commutes with the spin

$$[\hat{\mathbf{F}}_1^2, \hat{A}^\dagger] = 0, [\hat{\mathbf{F}}_2^2, \hat{B}^\dagger] = 0 \quad (31)$$

and it does not change total spin and any spin components but just add two particles. Therefore, we can construct the unnormalized spin state for  $N$  particles [11]: first, write down a state with necessary spin for a small number of particles; second, apply  $\hat{A}^\dagger (\hat{B}^\dagger)$  as many times as needed to get the desired number of particles. We got

$$|\otimes\rangle = Z^{1/2} (\hat{a}_1^\dagger)^{S_1} (\hat{b}_1^\dagger)^{S_2} (\hat{A}^\dagger)^{T_1} (\hat{B}^\dagger)^{T_2} |0\rangle \quad (32)$$

with the fixed number in the two sites satisfied  $T_{1,2} = (N_{1,2} - S_{1,2})/2$ .

For the region  $\Lambda > \frac{(2N-1)C_2}{C_1(N+1)}$ , if we let  $|N, N, 0, 0\rangle = Z^{1/2}(\hat{Q}^\dagger)^{2N}|0\rangle$ , the ground state for the Hamiltonian (9) is

$$|Q\rangle = Z^{1/2}(\hat{a}_1^\dagger)^S(\hat{b}_1^\dagger)^S(\hat{Q}^\dagger)^{2N-2S}|0\rangle \quad (33)$$

In the  $\Lambda < \frac{(2N-1)C_2}{C_1N}$  region, the system is polarized to the ferromagnetic phase, the ground state is

$$|P\rangle = Z^{1/2}(\hat{a}_1^\dagger)^{N_1}(\hat{b}_1^\dagger)^{N_2}|0\rangle. \quad (34)$$

#### IV. CONCLUSION

To summarize, we study the ground spin state of polar atoms ( $^{23}\text{Na}$ ) in the optical lattice subject to a magnetic

dipole-dipole interaction between nearby wells. We consider the special case that there are two particles per well, and show a new singlet state. In two well model, three kinds of spin ground state with total spin vanished ( $\hat{\mathbf{F}}^2 = \langle (\hat{\mathbf{F}}_1 \cdot \hat{\mathbf{F}}_2)^2 \rangle = 0$ ) are discussed and can be distinguished by the number fluctuations. The final states can be constructed by singlet pair creation operator and the quaternary-singlet creation operator.

- 
- [1] D. M. Stamper-Kurn, M. R. Andrews, A. P. Chikkatur, S. Inouye, H.-J. Miesner, J. Stenger, and W. Ketterle, Phys. Rev. Lett. **80**, 2027 (1998).
  - [2] J. Stenger et al., Nature (London) **396**, 345 (1998).
  - [3] M.-S. Chang, C. D. Hamley, M. D. Barrett, J. A. Sauer, K.M. Fortier, W. Zhang, L. You, and M. S. Chapman, Phys. Rev. Lett. **92**, 140403 (2004).
  - [4] Tin-Lun Ho, Phys. Rev. Lett. **81**, 742 (1998).
  - [5] T. Ohmi and K. Machida, J. Phys. Soc. Jpn. **67**, 1822 (1998).
  - [6] D. Jaksch et al., Phys. Rev. Lett. **81**, 3108 (1998).
  - [7] M.P.A. Fisher et al., Phys. Rev. B **40**, (1989).
  - [8] C. Orzel et al., Science **291**, 2386 (2001).
  - [9] M. Greiner et al., Nature (London) **415**, 39 (2002).
  - [10] E. Demler and F. Zhou, Phys. Rev. Lett. **88**, 163001 (2002).
  - [11] A. Imambekov, M. Lukin, and E. Demler, Phys. Rev. A **68**, 063602 (2003).
  - [12] S.K. Yip, Phys. Rev. Lett. **90**, 250402 (2003).
  - [13] S.K. Yip, J. Phys. B: Cond. Mat., **15**, 4583 (2003).
  - [14] M. Rizzi, D. Rossini, G. De Chiara, S. Montangero, and R. Fazio, Phys. Rev. Lett. **95**, 240404 (2005).
  - [15] F. Zhou and G.W. Semenoff, Phys. Rev. Lett. **97**, 180411 (2006).
  - [16] New Journal of Physics **9** (2007) 133.
  - [17] K. Goral et al., Phys. Rev. A **61**, 051601 (2000).
  - [18] L. Santos et al., Phys. Rev. Lett. **85**, 1791 (2000).
  - [19] S. Yi and L. You, Phys. Rev. A **63**, 053607 (2001).
  - [20] H. Pu, W. Zhang, and P. Meystre, Phys. Rev. Lett. **87**, 140405 (2001).
  - [21] H. Pu, W. Zhang, and P. Meystre, Phys. Rev. Lett. **89**, 090401 (2002).
  - [22] S. Yi and H. Pu, Phys. Rev. Lett. **97**, 020401 (2006); S. Yi and H. Pu, Phys. Rev. A **73**, 061602(R) (2006); S. Yi and H. Pu, Phys. Rev. A **73**, 023602 (2006).
  - [23] B. Sun, W. X. Zhang, S. Yi, M. S. Chapman, and L. You, Phys. Rev. Lett. **97**, 123201 (2006); Phys. Rev. Lett. **97**, 139902 (2006).
  - [24] S. Yi, T. Li, and C. P. Sun, Phys. Rev. Lett. **98**, 260405 (2007).
  - [25] C. K. Law, H. Pu, and N. P. Bigelow, Phys. Rev. Lett. **81**, 5257 (1998).
  - [26] T.-L. Ho and S.-K. Yip, Phys. Rev. Lett. **84**, 4031 (2000).
  - [27] H. Pu, C. K. Law, S. Raghavan, J. H. Eberly, and N. P. Bigelow, Phys. Rev. A **60**, 1463 (1999); H. Pu, S. Raghavan, and N. P. Bigelow, ibid. **61**, 023602 (2000).
  - [28] S. Yi, O. E. Mu, tecaplioglu, C. P. Sun, and L. You, Phys. Rev. A **66**, 011601(R) (2002).
  - [29] W. Zhang, H. Pu, C. Search, and P. Meystre, Phys. Rev. Lett. **88**, 060401 (2002).
  - [30] S. Giovanazzi, D. O'Dell, and G. Kurizki, Phys. Rev. Lett. **88**, 130402 (2002).
  - [31] M. Koashi and M. Ueda, Phys. Rev. Lett. **84**, 1066 (2000).
  - [32] M. Ueda and M. Koashi, Phys. Rev. A **65**, 063602 (2002).
  - [33] M. Luo, Z. B. Li, and C. G. Bao, Phys. Rev. A **75**, 043609 (2007).
  - [34] Z. F. Xu, Y. Zhang, and L. You, Phys. Rev. A **79**, 023613 (2009).
  - [35] Z. F. Xu, J. Zhang, Y. Zhang, and L. You, Phys. Rev. A **81**, 033603 (2010).
  - [36] J. Zhang, Z. F. Xu, L. You and Y. Zhang, Phys. Rev. A **82**, 013625 (2010).
  - [37] J. Zhang, T. T. Li, Y. Zhang, Phys. Rev. A **83**, 023614 (2011).
  - [38] Y. Shi, Phys. Rev. A **82**, 023603 (2010).
  - [39] Y. Shi and L. Ge, Phys. Rev. A **83**, 013616 (2011).
  - [40] S. K. Yip, Phys. Rev. Lett. **90**, 250402 (2003).
  - [41] Masato Koashi and Masahito Ueda, Phys. Rev. Lett. **84**, 1066 (2000).
  - [42] Ying Wu, Phys. Rev. A **54**, 4534 (1996).